Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 1.12

Global applicability domain: Inside

Local applicability domain index: 7.94e-01

Confidence level: 7.10e-01

Nearest Neighbors from the Training Set

Image not found
N,N-Dimethylformamide
Measured: 7.94e-01
Predicted: 1.12

Image not found
Morpholine
Measured: 2.82
Predicted: 1.87

Image not found
1,4-Dioxane
Measured: 5.01e-01
Predicted: 1.06

Image not found
Piperazine
Measured: 3.89
Predicted: 2.44

Image not found
Ethylene thiourea
Measured: 1.82
Predicted: 1.85